PROPAGATION OF NUCLEAR DATA UNCERTAINTIES IN FUEL CYCLE CALCULATIONS USING MONTE-CARLO TECHNIQUE

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Abstract

The **uncertainty propagation** in fuel cycle calculations **due to Nuclear Data** (ND) is a important issue for :

- Present fuel cycles (e.g. high burnup fuel programme)
- New fuel cycles designs (e.g. fast breeder reactors and ADS)

Different error propagation techniques can be used:

- Sensitivity analysis
- Response Surface Method
- **Monte Carlo technique**

Then, in this paper, it is assessed the **impact of ND uncertainties on the decay heat and radiotoxicity in two applications:**

- Fission Pulse Decay Heat calculation (**FPDH**)
- Conceptual design of European Facility for Industrial Transmutation (**EFIT**)

The complete set of **uncertainty data** for **cross sections** (EAF2007/UN), **decay data** and **fission yield data** (JEFF-3.1.1) are processed and used in **ACAB code**.

OUTLINE

PART I: **Methodology to propagate ND uncertainties using Monte Carlo technique**

PART II: **Application of Monte Carlo technique**

A. Fission Pulse Decay Heat calculation

B. EFIT fuel cycle calculation

CONCLUSIONS

Goal: "To analyse how ND uncertainties are transmitted to response functions"

$$\boxed{\frac{dN}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\cdot \Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\cdot \Phi N = A \cdot N} \Longrightarrow N_i = N_i(\lambda, \sigma, \gamma)$$

1) <u>Sensitivity / Uncertainty Analysis (S/U)</u>
   - First order Taylor series (**linear approximation**)

2) **<u>Monte Carlo Uncertainty Analysis (MC)</u>**
   - To treat the global effect of all nuclear data uncertainties
   - Without any approximation

Monte Carlo technique

- Individual / All together sampling (λ, σ, γ)
- PDFs

Normal distribution

$$\sigma_j \rightarrow N[\sigma_{j0}, DST(\sigma_j)] \Rightarrow \varepsilon_j \rightarrow N(0, \Delta_j)$$

$$\boxed{\Rightarrow \text{If } \uparrow\uparrow \Delta_j \Rightarrow \text{Maybe } \sigma_j < 0}$$

LogNormal distribution

$$\boxed{\text{Always } \sigma_i > 0}$$

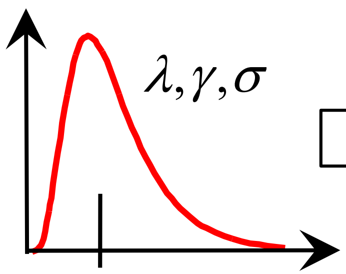
$$\boxed{\log\begin{pmatrix} (\sigma_1/\sigma_{10}) \\ \vdots \\ (\sigma_m/\sigma_{m0}) \end{pmatrix} \rightarrow N(0, M)}$$

Nuclear Data libraries Collapsed

Mean Values

Uncertainties (Standard Desv)

LogNormal distribution



λ, γ, σ

Samplig	ACAB	Results
$\lambda_1, \gamma_1, \sigma_1$	$\longrightarrow$	N_1
$\lambda_2, \gamma_2, \sigma_2$	$\longrightarrow$	N_2
...		...
$\lambda_n, \gamma_n, \sigma_n$	$\longrightarrow$	N_n

Uncertainty data

➔ Cross section from activation-oriented nuclear data libraries

- EAF2007-UN

e.g.: $W^{180}(n,\gamma)$

E_{i+1}(eV)

```
W -180N,G                                                                748033102
 7.41800E+4 1.7840E+02          0          0          0              1748033102
 0.0000E+00 0.0000E+00          0        102          0              1748033102
 0.0000E+00 0.0000E+00          0          1         10              5748033102
 1.0000E-05 1.0000E+00 5.0000E+00 1.8404E-01 1.0140E+02 2.5000E-01748033102
 2.0000E+07 2.5000E-01 6.0000E+07 0.0000E+00                          748033102
```

E_i (eV)

$\Delta^2_{I=1,EAF}$ (relative error, Δ)~ $\Delta_{I=1,EXP}$= $\Delta_{I=1,EAF}/3$

➔ Fission yield from evaluated nuclear data library

- JEFF 3.1.1

$\gamma_{Th232 \rightarrow H3, 400KeV} + 1\sigma_\gamma$

Th232

400 KeV

H3

```
 9.023200+4 2.300450+2          2          0          0          03486 8454    1
 4.0000E+05 0.0000E+00          1          0       3664          9163486 8454    2
 1.0010E+03 0.0000E+00 1.6073E-05 5.5423E-06 1.0020E+03 0.0000E+003486 8454    3
 4.9121E-06 1.6564E-06 1.0030E+03 0.0000E+00 7.0081E-05 2.2139E-053486 8454    4
```

Processing and collapsing of nuclear data

<u>Collapsing method:</u>

-<u>Cross section:</u> Conservation of reaction rate

$$\boxed{Rate_{j\to i} = \int_E \sigma_{j\to i}(E)\cdot\phi(E)\cdot dE = \sigma_{j\to i}^{eff}\cdot\phi_T}$$

-<u>Uncertainties:</u> Using **Sandwich rule** (*Propagation of Momentum, first order)*

$$\Delta^2 = \omega^T V \omega$$

H. Hiruta *et al.* , "*Few Group Collapsing of Covariance Matrix Data Based on a Conservation Principle*", Nuclear Data Sheets, vol. 109, 2801-2806, (Dec 2008)

Collapsing without losing information

Processing and collapsing of nuclear data

➔ Cross section

Given ***V*** the G-by-G variance matrix of the relative cross sections vector, the variance Δ^2 of the relative spectrum-averaged cross section is: $\Delta^2 = \omega^T V \omega$

with $\omega = [\frac{\phi_1}{\bar{\phi}} \frac{\sigma_1}{\sigma^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}} \frac{\sigma_G}{\sigma^{eff}}]^T$

$$\bar{\phi} = \phi_1 + \phi_2 + \cdots + \phi_G$$

$$\sigma^{eff} = \frac{\phi_1\sigma_1 + \phi_2\sigma_2 + \cdots + \phi_G\sigma_G}{\phi_1 + \phi_2 + \cdots + \phi_G}$$

➔ Fission yield

Given **G** the M-by-M variance matrix of the relative fission yield vector, the variance Δ^2 of the relative spectrum-averaged fission yield is: $\Delta^2 = \omega^T G \omega$

with $\omega = [\frac{\phi_1}{\bar{\phi}} \frac{\sigma_{1,fiss}}{\sigma_{fiss}^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}} \frac{\sigma_{G,fiss}}{\sigma_{fiss}^{eff}}]^T$ where $\gamma_{j,i}^{eff} = \frac{\gamma_1^{j,i}\sigma_1^{fiss,j}\phi_1 + \ldots + \gamma_G^{j,i}\sigma_G^{fiss,j}\phi_G}{\sigma_1^{fiss,j}\phi_1 + \ldots + \sigma_G^{fiss,j}\phi_G}$

Advantages & Disadvantages of Monte Carlo Technique

➔ **Advantages**

- Collapsing to one energy group → Reduce amount of variables to sample
- No sensitivity coefficients should be calculated
- No approximation on equations → Take into account non-linear effects

➔ **Disadvantages**

- How to check if the phase space is well sampled ?
- Which PDFs should be taken ?
- Computational demanding

APPLICATIONS:

A. Fission Pulse Decay Heat calculation

B. EFIT fuel cycle calculation

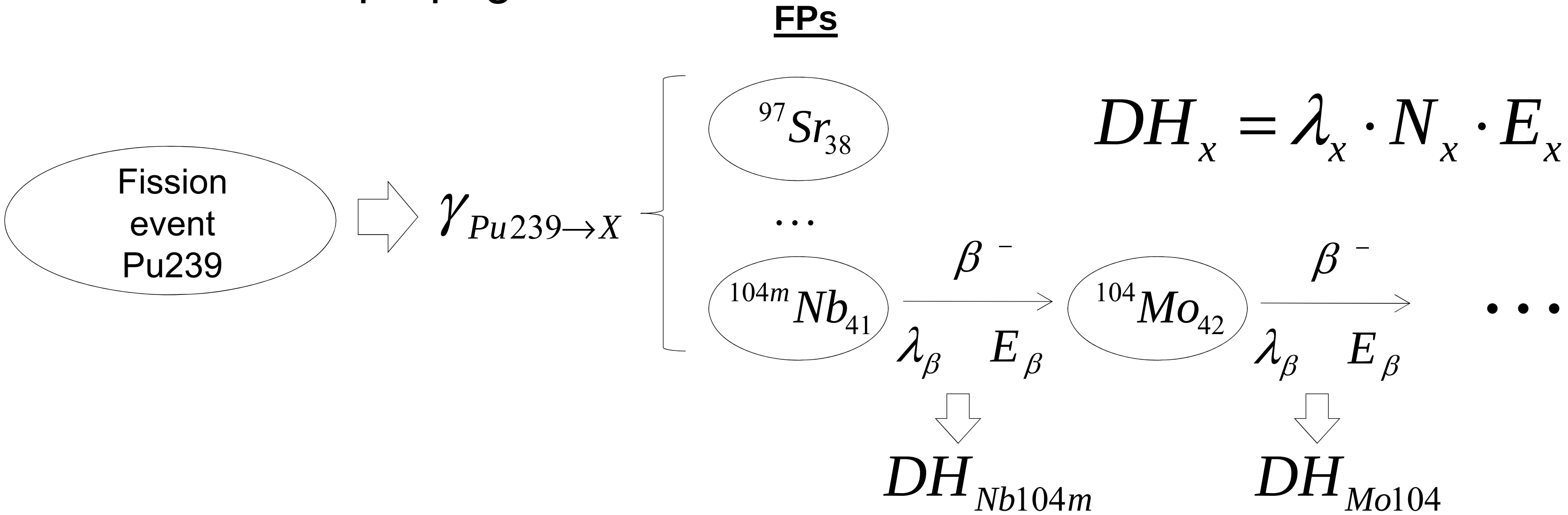
A. Fission Pulse Decay Heat calculation

Description of the problem

- **Decay heat** of a **single thermal fission event in Pu239**
- Isotopes: **only Fission Products** (FPs)
- Only **Fission yield (FY) and Decay data** (Energy/Decay constant)

uncertainties are propagated

$$DH_x = \lambda_x \cdot N_x \cdot E_x$$



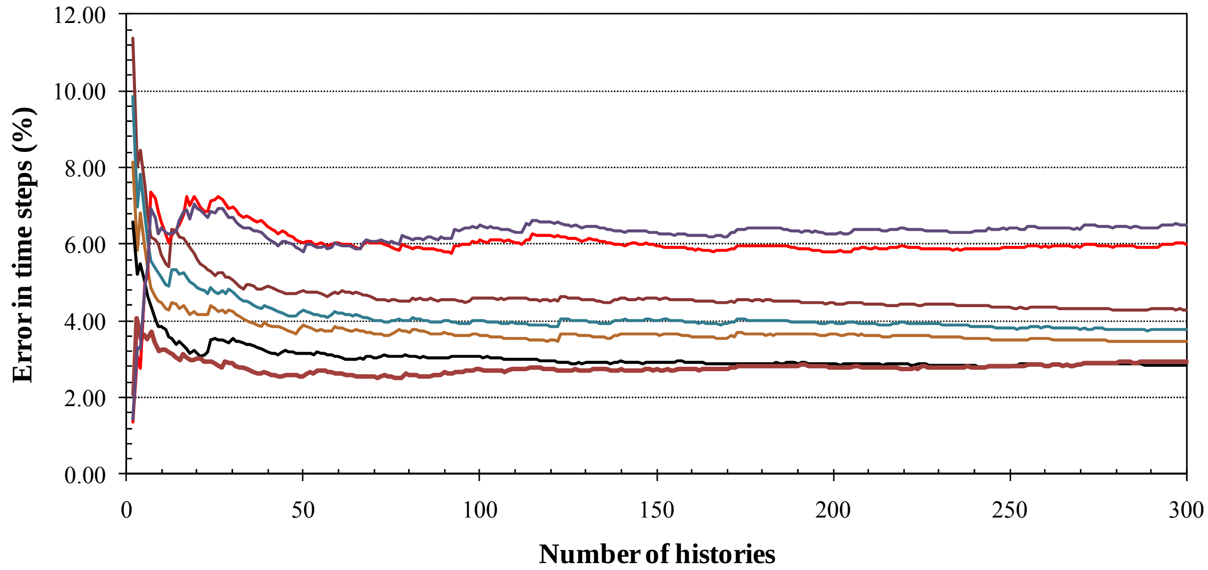
Calculations

- Histories launched/case: 300

- Relative error followed

Case studied

- Total decay heat
- Beta decay heat
- Gamma decay heat



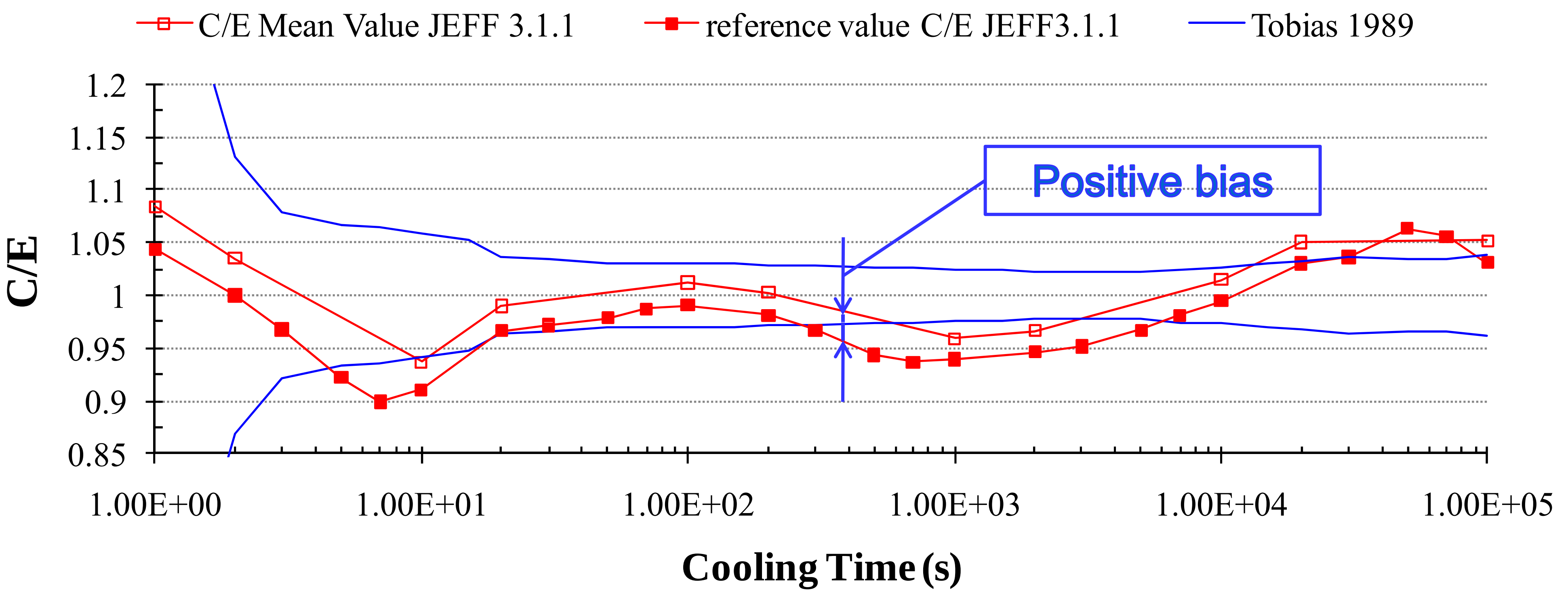
Only known uncertainties // All with uncertainties

For unkown uncertainties

Decay Mode	Uncertainty
Alfa	10%
Beta	15%
Gamma	15%

Compared with:
- JEFF report 20
- Tobias exp. data

Total decay heat



B. EFIT fuel cycle calculation

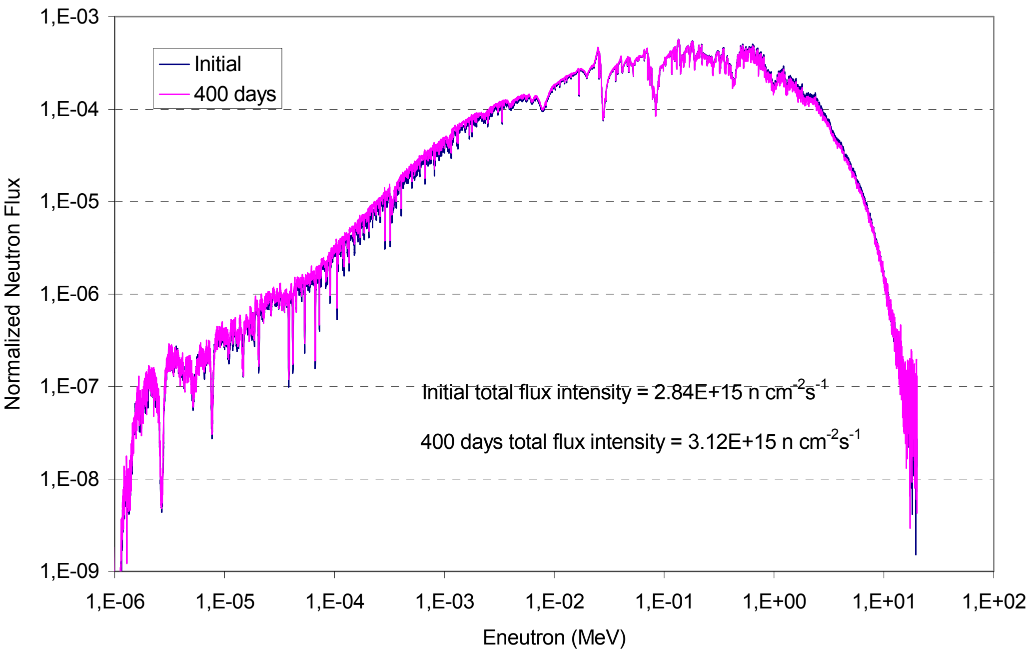
Reference system

- One of the preliminary conceptual designs of the **E**uropean **F**acility for **I**ndustrial **T**ransmutation (**EFIT**)

Coolant	**Pure Lead**
Thermal Power	**400 MWth**
Fuel	**(Pu, Am)O_2 + MgO**
Initial mass of actinides	**2.074 tonnes**

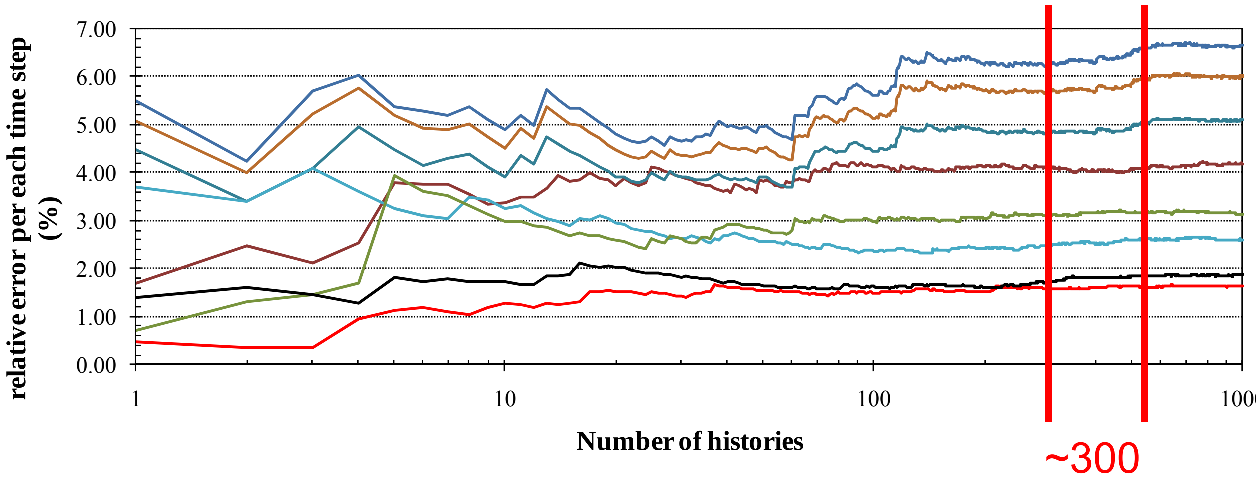
- **Constant neutron environment:**
  - neutron flux: 3.12 x 10^{15} n/cm^2 s
  - average energy <E> = 0.37 MeV

- **Calculations for discharge burn-up:**
  - 150 GWd/tHM (778 irradiation days)
  - 500 GWd/tHM (3225 irradiation days)



Calculations

- Histories launched:
  1000/DH case
  300/RTX case



Case studied

1. Decay heat
2. Radiotoxicity
   a. Inhalation dose
   b. Ingestion dose

All uncertainties are propagated:

- Individually
- All together

$\sigma, \quad \gamma, \quad \lambda$

Decay heat for *150 GWd/tHM*

Main contributors analysis

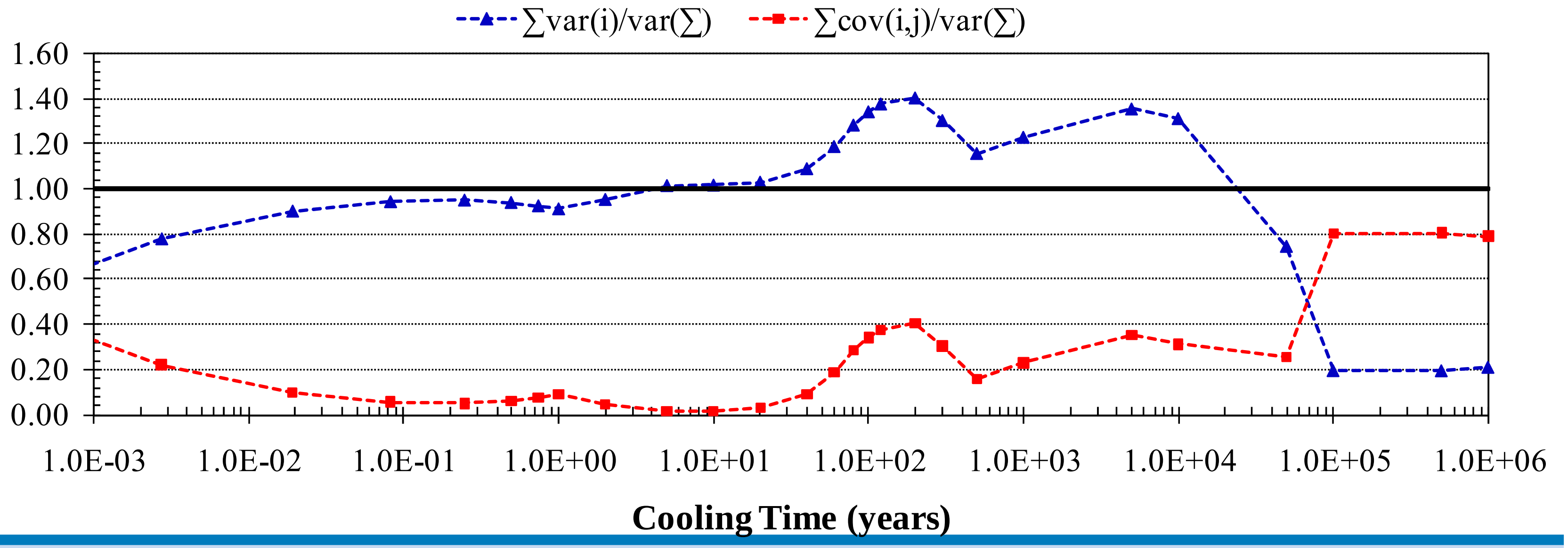
$$DH_{total} = \sum_{i=isotope} DH_i$$

$$\mathrm{var}(y) = \sum_{i=1}^{N} \mathrm{var}(y_i) + \sum_{i,j=1;i\neq j}^{N} \mathrm{cov}(y_i, y_j)$$

$$\Rightarrow$$

$$\sum_{i=1}^{N} \mathrm{var}(y_i) >> \sum_{i,j=1;i\neq j}^{N} \mathrm{cov}(y_i, y_j)$$

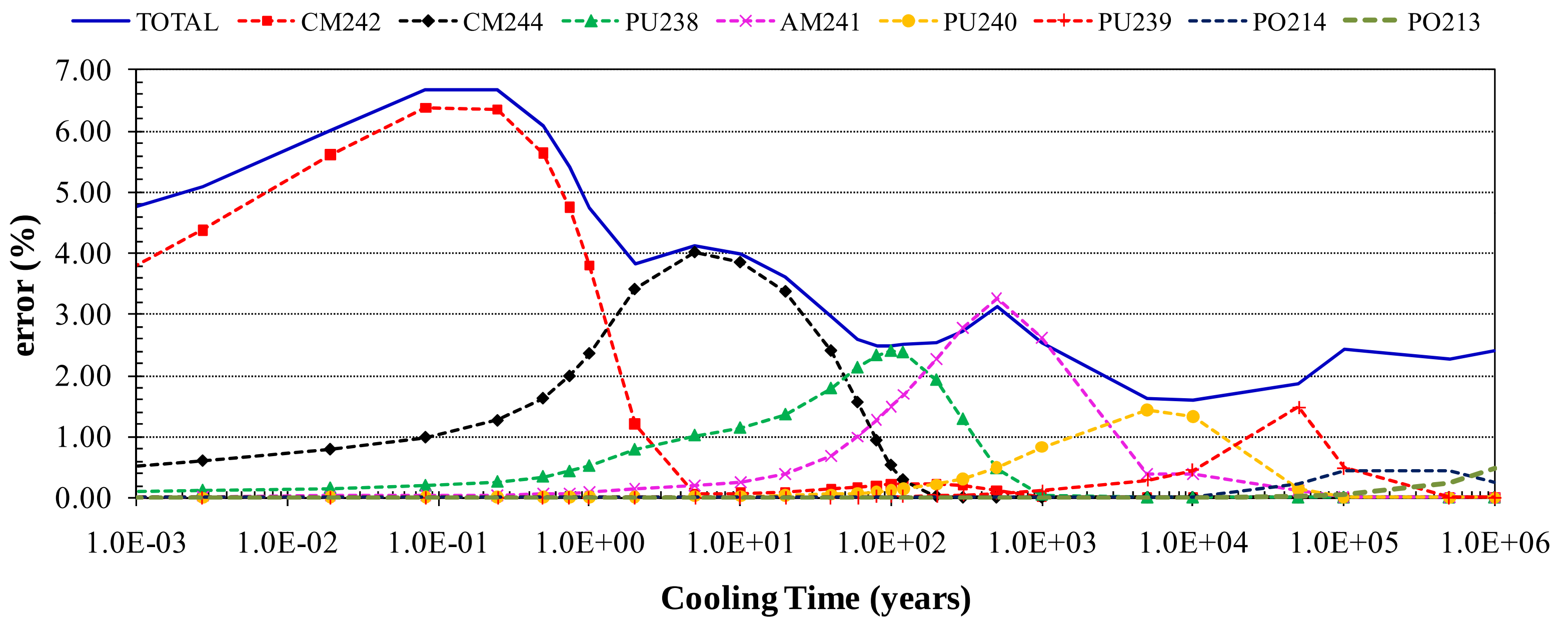
$$\frac{\sigma_x^2}{x^2} = \sum_{i=1}^{N} \frac{\sigma_{y_i}^2}{y_i^2} \cdot \frac{y_i^2}{x^2} = \sum_{i=1}^{N} error(y_i)^2 \cdot \frac{y_i^2}{x^2}$$



Decay heat for *150 GWd/tHM*

Main contributors

Cm242	Cm244	Pu238
Am241	Pu240	Pu239

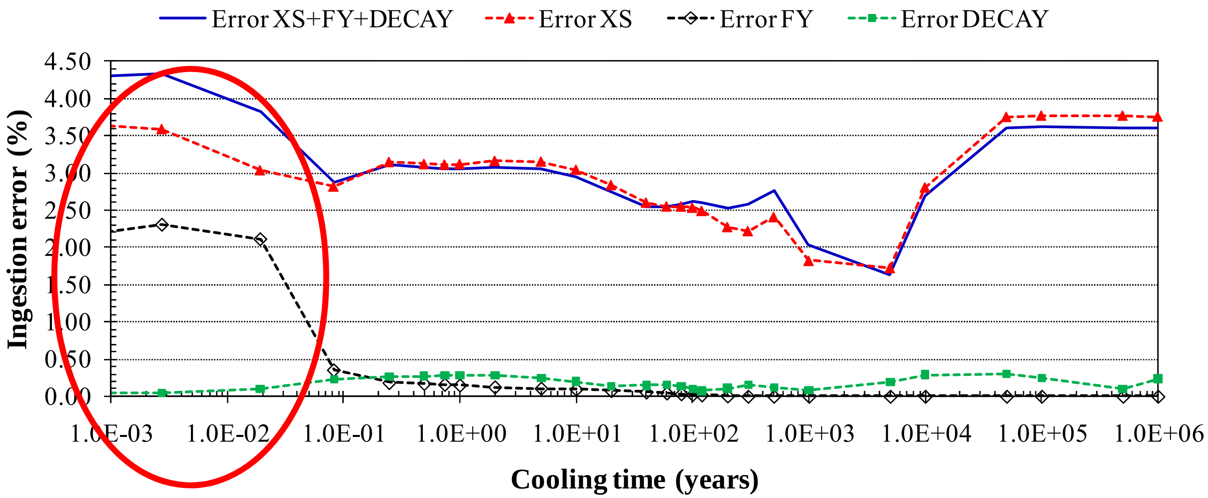


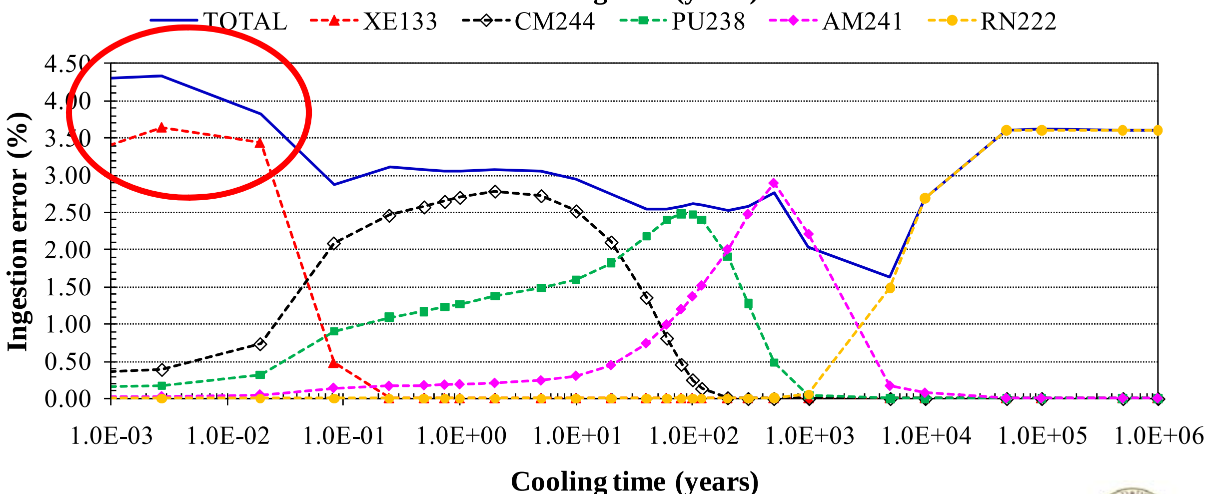
Radiotoxicity for *150 GWd/tHM*

Ingestion

Xe133	Cm244	Pu238
Am241	Rn222	

Due to FY / XS error





CONCLUSIONS

CONCLUSIONS

- **Monte Carlo technique for ND uncertainty propagation in activation calculations**
  - ***Pre-proccesing of nuclear data is needed:*** ***- Identifying uncertainties***
    - Collapsing of nuclear data
  - ***Implemented on ACAB code***
- **Monte Carlo technique** VS **deterministic calculations / experimental data**
  - ***A good agreement is found between both***
- A method to identify **main contributors to error** is developed based on MC results
- **PDFs dependency** is found in **FPDH calculation**, but **not in EFIT calculation**

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THANK YOU
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